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HIGH-ACCURACY MR-MP PERTURBATION THEORY ENERGY AND RADIATIVE RATES CALCULATIONS FOR CORE-EXCITED TRANSITIONS IN Fe XVI

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ABSTRACT

Accurate theoretical energy level, lifetime, and transition probability calculations of core-excited Fe XVI were performed employing the relativistic Multireference Møller–Plesset perturbation theory. In these computations the term energies of the highly excited $n \leqslant 5$ states arising from the configuration $1s^2 2s^k 2p^m 3\ell^p n\ell'^q$, where $k + m + p + q = 9$, $\ell \leqslant 3$ and $p + q \leqslant 2$ are considered, including those of the autoionizing levels with a hole-state in the L-shell. All even and odd parity states of sodium-like iron ion were included for a total of 1784 levels. Comparison of the calculated L-shell transition wavelengths with those from laboratory measurements shows excellent agreement. Therefore, our calculation may be used to predict the wavelengths of as of yet unobserved Fe XVI, such as the second strongest $2p$–$3d$ Fe XVI line, which has not been directly observed in the laboratory and which blends with one of the prominent Fe XVII lines.

Key words: atomic processes – line: formation – stars: coronae – Sun: X-rays, gamma rays – X-rays: general

Online-only material: machine-readable tables

1. INTRODUCTION

The complex spectra of highly charged multi-valence-electron ions of iron and nickel are observed in the solar corona, and they are prominent in many stellar coronae and other astrophysical plasmas, where they play an important role as diagnostics of plasma processes (Culhane & Acton 1974; Doschek & Feldman 2010; Paerels & Kahn 2003). The spectra produced by ions of these elements extend from the UV (and sometimes the visible) into the X-ray region. The L-shell X-ray emission lines from iron ions have become of particular interest, because they dominate many of the high-resolution grating spectra observed with the *Chandra* and *XMM-Newton* X-ray observatories (Canizares et al. 2000; Brinkman et al. 2001), and supporting laboratory measurements and improved calculations have been made to ascertain the spectral lines from these complex ions (Brown et al. 1998, 2002; Drake et al. 1999; Gu 2005; Kotochigova et al. 2007; Chen et al. 2007).

The discovery of absorption features in warm gas surrounding active galactic nuclei near 15–17 Å (Sako et al. 2001; Holczer et al. 2005) has provided additional impetus for studying iron L-shell X-ray spectra. In this case, the L-shell transitions in M-shell iron ions, i.e., core-excited transitions in iron ions that have a partially filled $n = 3$ shell, are of special interest.

L-shell transitions in M-shell iron ions have typically been ignored in the spectra from collisional sources as being too weak to be important. The L-shell emission from Na-like Fe XVI, however, has been an exception. Three such lines were included in the modeling of the spectrum from Capella (Behar et al. 2001), which showed them to be weak. However, the concurrent discovery that Fe XVI lines could blend with Fe XVII lines and drastically alter the prominent Fe XVII line ratios (Brown et al. 2001) resulted in much interest in the L-shell transitions from Fe XVI, including detailed modeling of their contributions to solar X-ray spectra (Brickhouse & Schmelz 2006). Dielectronic recombination may also contribute to the emission of core-excited Fe XVI lines, and Fe XVI features produced by this process have now been identified in the grating-spectrometer observations of Capella (Beiersdorfer et al. 2011), where they have been used to derive the electron temperature associated with the Fe XVII emission.

Because the energy required to excite an L-shell X-ray transition in Fe XVI (about 800 eV) is higher than the ionization potential of Na-like Fe^{15+}, it is difficult to observe collisionally excited Fe XVI lines in the laboratory. Most Fe XVI lines observed in the laboratory have been from high-density spark or laser-produced plasma source excited by dielectronic recombination (Burkhalter et al. 1979; May et al. 2005). An exception is the work by Graf et al. (2009), who made high-resolution grating spectrometer measurements of collisionally excited L-shell X-ray lines of Fe XVI. These measurements have high accuracy and can be used to evaluate calculations.

While several authors published theoretical studies on the structure of the one-valence-electron Na-like Fe XVI system (Aggarwal & Keenan 2007; Kisielius et al. 2003; Buchet et al. 1980), theoretical studies of the core-excited levels of Fe XVI are sparse. Variational methods like multiconfigurational Hartree–Fock (MCHF), multiconfigurational Dirac–Fock (MCDF) and configuration-interaction (CI) methods are relatively efficient for few-valence-electron systems. However, they have difficulties when applied to the calculation of energy levels with electron holes in the core. To account for core-valence correlation effects, very large sets of configuration state functions (CSFs) have to be employed. In the Na-like systems, a $2s$ or $2p$ electron of the $2s^2 2p^6$ core may be placed into a $3s$, $3p$, $3d$, $4s$, $4p$, or higher valence shell. Moreover, intermediate coupling must be used because neither the LS-coupling nor the jj-coupling approach is appropriate.

During the past decade there have been several theoretical developments to obtain wavelengths that closely match those produced by laboratory measurements and required by high-resolution astrophysical observations. For example, Safronova et al. (2002b) utilized the relativistic many-body perturbation theory (MBPT) method to calculate the Na-like Fe XVI energy

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levels. Similarly, Gu (2005) and Gu et al. (2006) implemented a combination of the MBPT method and the CI method to produce wavelengths of L-shell transitions in iron and nickel that were shown to be superior to earlier results using the CI method alone, as employed, for example, by the flexible atomic code (FAC; Gu 2008).

In the following, we employ another recently developed method for performing accurate energy level calculations: the relativistic Multireference Møller–Plesset (MR-MP) perturbation theory (Ishikawa et al. 1991; Vilkas & Ishikawa 2003b). This approach has also been shown to produce very accurate wavelengths. As an example, we can mention the transition energies calculated with this method for the L-shell transitions of Fe XVII (Ishikawa et al. 2009), which where found to agree with measurements within the experimental uncertainties. This method has also been used to calculate a limited set of Fe XVI transitions (Beiersdorfer et al. 2012), which achieved excellent agreement with the laboratory data of Graf et al. (2009). Here, we extend these calculations to core-excited levels with valence electrons in the $n = 3, 4, 5$ shell, and we give values for the radiative decay rates and the associated radiative level lifetimes.

2. METHODS

2.1. Relativistic Multireference Many-body Perturbation Theory

The effective N-electron Hamiltonian for the development of our relativistic MR-MP algorithm is taken to be the relativistic "no-pair" Dirac–Coulomb–Breit (DCB) Hamiltonian $H^{+}_{\rm DCB}$ (Sucher 1980; Mittleman 1981). Second-order variation of the state-averaged energy ($\Omega_{\rm state\text{-}ave}$),

$$\Omega_{\rm state\text{-}ave} = \sum_{\gamma_K \mathcal{J}\pi} \sum_{IJ}^{\mathfrak{P}(+)} C_{IK} C_{JK} \left\langle \Phi_I^{(+)}(\gamma_I \mathcal{J}\pi) | H^{+}_{\rm DCB} | \Phi_J^{(+)}(\gamma_J \mathcal{J}\pi) \right\rangle, \quad (1)$$

is taken with respect to the matrix elements of spinor unitary rotation matrix and configuration mixing coefficients $\{C_{IK}\}$ in the state-average multiconfiguration Dirac–Fock–Breit self-consistent field (MCDFB SCF) wave function,

$$\psi_K^{\rm MC}(\gamma_K \mathcal{J}\pi) = \sum_{I}^{\mathfrak{P}(+)} C_{IK} \Phi_I^{(+)}(\gamma_I \mathcal{J}\pi), \quad (2)$$

leading to the Newton–Raphson equations for second-order MCDFB SCF wave functions (Vilkas et al. 1998). The summation indices $\mathcal{J}$, π, and γ run over the ground and excited states. These indices represent the total angular momentum ($\mathcal{J}$), parity (π), and the quantum number (γ) essential to uniquely specify the state. This state-averaged second-order MCDFB equation yields a well balanced set of spinors suitable for describing the ground and low-lying even- and odd-parity excited (γ, $\mathcal{J}$, π) levels. For the sodium-like ions, the state-averaged MCDFB SCF includes a total of 21 CSFs of even and odd parity with $\mathcal{J} = 1/2 - 7/2$, $\{\Phi_I^{(+)}(\gamma_I \mathcal{J}\pi) \in \mathfrak{P}^{(+)}\}$,where $\mathfrak{P}^{(+)}$ means positive-energy space, arising from the $1s^2 2s^2 2p^6 3s^1$ through $1s^2 2s^2 2p^6 5f^1$ configurations. In particular, we consider single excitation of an electron from the $3s$ to $n\ell$ shell, where $n = \{3, 4, 5\}$ and $\ell = \{s, p_{1/2}, p_{3/2}, d_{3/2}, d_{5/2}, f_{5/2}$, and $f_{7/2}\}$. In addition we included two CSFs with core excitation of an electron from $2p_{1/2}$ and $2p_{3/2}$ to $3s$. Using the V^{N-n} method, we determine a single set of spinors via the state-averaged MCDFB SCF wave functions, which is crucial to implement a "high-accuracy" algorithm for multi-valence electron systems. As a result, a well balanced description of the ground and excited levels is obtained (Dzuba 2005).

In order to account for strong configuration mixing among the quasi-degenerate open-shell states, a multireference configuration interaction (MR-CI) calculation for the ground and low-lying excited $\mathcal{J} = 1/2 - 11/2$ states in the sodium-like ions was subsequently carried out, which included a total of 1784, even- and odd-parity CSFs arising from the configurations $2s^k 2p^m 3\ell^p n\ell'^q$, with $k + m + p + q = 9$, $n = \{3, 4, 5\}$, and $p + q \leqslant 2$. Variation of the configuration-state coefficients $\{C_{IK}\}$ leads to the determinantal CI equation,

$$\det\Big[\left\langle \Phi_I^{(+)}(\gamma_I \mathcal{J}\pi) | H^{+}_{\rm DCB} | \Phi_J^{(+)}(\gamma_I \mathcal{J}\pi) \right\rangle - E^{\rm CI} \left\langle \Phi_I^{(+)}(\gamma_I \mathcal{J}\pi) | \Phi_J^{(+)}(\gamma_I \mathcal{J}\pi) \right\rangle\Big] = 0 \quad (3)$$

The eigenfunctions $\psi_K^{\rm CI}(\gamma_K \mathcal{J}\pi)$ form a CI subspace $\mathfrak{P}_{\rm CI}^{(+)}$ of the positive-energy space $\mathfrak{D}^{(+)}$,

$$\psi_K^{\rm CI}(\gamma_K \mathcal{J}\pi) = \sum_{I}^{M_{\rm CI}} C_{IK} \Phi_I^{(+)}(\gamma_I \mathcal{J}\pi),\ K = 1, 2, \ldots M_{\rm CI} \left(\in \mathfrak{P}_{\rm CI}^{(+)}\right). \quad (4)$$

Table 1
Energies (in $\rm cm^{-1}$) of the $1s^2 2s^2 2p^6\ n\ell$ Levels ($n \leqslant 5$, $\ell \leqslant 3$) in Fe XVI

Configuration	J(Index)Parity	Energy[a]	Energy[b]	NIST[c]	Δ
$3s^1$	1/2(1)	0	0	0	0
$3p^1_{1/2}$	1/2(1)*	277210	277222 [12]	277194	28
$3p^1_{3/2}$	3/2(1)*	298162	298167 [5]	298143	24
$3d^1_{3/2}$	3/2(1)	675468	675463 [5]	675501	−38
$3d^1_{5/2}$	5/2(1)	678378	678372 [6]	678406	−34
$4s^1$	1/2(2)		1867664	1867740	−76
$4p^1_{1/2}$	1/2(2) *		1977616	1977650	16
$4p^1_{3/2}$	3/2(2) *		1985786	1985650	136
$4d^1_{5/2}$	3/2(2)		2124584	2124720	−136
$4d^1_{7/2}$	5/2(2)		2125923	2125660	263
$4f^1_{5/2}$	5/2(1) *		2184910	2184960	−50
$4f^1_{7/2}$	7/2(1) *		2185401	2185410	−9
$5s^1$	1/2(3)		2663328	2662000	1328
$5p^1_{1/2}$	1/2(3) *		2717620	2717170	450
$5p^1_{3/2}$	3/2(3) *		2721636	2721160	476
$5d^1_{5/2}$	3/2(3)		2788713	2788050	663
$5d^1_{5/2}$	5/2(3)		2789416	2788610	806
$5f^1_{5/2}$	5/2(2) *		2818974	2818600	374
$5f^1_{7/2}$	7/2(2) *		2819226	2818900	326

Notes. Numbers in brackets show the difference ($\rm cm^{-1}$) between MR-MP calculations that considered only up to $n = 3$. In the last column we included the energy difference (Δ) with NIST (in $\rm cm^{-1}$). The energy-ordered level index for a given level with total angular momentum J and parity is given in parentheses. An asterisk (∗) denotes odd parity configurations; the lack thereof denotes an even parity configuration.

[a] Derived from MR-MP calculations that included only $n \leqslant 3$ excited levels Beiersdorfer et al. (2012).

[b] Present calculation.

[c] Kramida et al. (2012). NIST Atomic Spectra Database (ver. 5.0), [Online]. Available: http://physics.nist.gov/asd [2012 November 21]. National Institute of Standards and Technology, Gaithersburg, MD.

(This table is available in its entirety in a machine-readable form in the online journal. A portion is shown here for guidance regarding its form and content.)

Table 2
Energies (in cm^{-1}) of the First 67 MR-MP Calculated Core Configurations $1s^2 2s^2 2p^1_{1/2} 2p^4_{3/2} 3\ell^p 3\ell'^q$, ($\ell \leqslant 2$, and $p+q=2$) in Fe XVI

Configuration	J(Index)Parity	Energy	Configuration	J(Index)Parity	Energy
$3s^2$	1/2(4) *	5857665	$3p^1_{1/2}3d^1_{5/2}$	5/2(20)	6799158
$3s^1 3p^1_{1/2}$	1/2(6)	6077192	$3p^1_{3/2}3d^1_{5/2}$	5/2(21)	6804620
$3s^1 3p^1_{1/2}$	1/2(7)	6082835	$3p^1_{1/2}3d^1_{5/2}$	3/2(22)	6806274
$3s^1 3p^1_{1/2}$	3/2(7)	6087509	$3p^1_{3/2}3d^1_{3/2}$	3/2(23)	6812168
$3s^1 3p^1_{3/2}$	3/2(8)	6100268	$3p^1_{3/2}3d^1_{3/2}$	1/2(17)	6813392
$3s^1 3p^1_{3/2}$	5/2(7)	6108077	$3p^1_{3/2}3d^1_{5/2}$	7/2(12)	6814230
$3s^1 3p^1_{3/2}$	1/2(8)	6182346	$3p^1_{3/2}3d^1_{5/2}$	5/2(22)	6815936
$3s^1 3p^1_{3/2}$	3/2(10)	6201702	$3p^1_{1/2}3d^1_{3/2}$	3/2(25)	6831282
$3s^1 3p^1_{1/2}$	1/2(9)	6245187	$3p^1_{1/2}3d^1_{3/2}$	1/2(18)	6841603
$3p^2_{1/2}$	1/2(7) *	6362006	$3p^1_{3/2}3d^1_{3/2}$	3/2(26)	6859383
$3p^1_{1/2}3p^1_{3/2}$	3/2(10) *	6390640	$3p^1_{3/2}3d^1_{3/2}$	1/2(20)	6878831
$3p^1_{1/2}3p^1_{3/2}$	5/2(7) *	6394058	$3p^1_{3/2}3d^1_{3/2}$	7/2(13)	6884423
$3p^1_{1/2}3p^1_{3/2}$	1/2(9) *	6398771	$3p^1_{3/2}3d^1_{3/2}$	5/2(24)	6888882
$3p^2_{3/2}$	3/2(13) *	6422064	$3p^1_{3/2}3d^1_{5/2}$	3/2(27)	6894592
$3p^2_{3/2}$	5/2(9) *	6423498	$3p^1_{1/2}3d^1_{3/2}$	1/2(21)	6913088
$3s^1 3d^1_{5/2}$	3/2(15) *	6483365	$3p^1_{1/2}3d^1_{3/2}$	3/2(28)	6920217
$3s^1 3d^1_{3/2}$	3/2(16) *	6502061	$3p^1_{1/2}3d^1_{5/2}$	5/2(25)	6926090
$3s^1 3d^1_{5/2}$	5/2(11) *	6504077	$3d^1_{3/2}3d^1_{5/2}$	7/2(15) *	7165078
$3p^2_{3/2}$	1/2(12) *	6508883	$3d^2_{5/2}$	9/2(5) *	7172806
$3p^2_{1/2}$	1/2(13) *	6514341	$3d^1_{3/2}3d^1_{5/2}$	3/2(28) *	7183471
$3s^1 3d^1_{5/2}$	5/2(13) *	6514575	$3d^2_{5/2}$	7/2(16) *	7185214
$3s^1 3d^1_{5/2}$	7/2(8) *	6514871	$3d^1_{3/2}3d^1_{5/2}$	5/2(23) *	7186088
$3s^1 3d^1_{5/2}$	3/2(18) *	6550184	$3d^2_{3/2}$	5/2(24) *	7193832
$3s^1 3d^1_{3/2}$	1/2(14) *	6573657	$3d^1_{3/2}3d^1_{5/2}$	3/2(29) *	7203616
$3s^1 3d^1_{5/2}$	5/2(14) *	6593543	$3d^1_{3/2}3d^1_{5/2}$	1/2(21) *	7204117
$3s^1 3d^1_{5/2}$	3/2(19) *	6616740	$3d^1_{3/2}3d^1_{5/2}$	9/2(6) *	7209123
$3p^1_{1/2}3d^1_{3/2}$	5/2(16)	6735550	$3d^2_{5/2}$	5/2(25) *	7211689
$3p^1_{1/2}3d^1_{3/2}$	5/2(17)	6743324	$3d^2_{5/2}$	1/2(23) *	7235908
$3p^1_{1/2}3d^1_{5/2}$	7/2(9)	6756215	$3d^1_{3/2}3d^1_{5/2}$	7/2(17) *	7242818
$3p^1_{1/2}3d^1_{5/2}$	5/2(18)	6760746	$3d^1_{3/2}3d^1_{5/2}$	5/2(26) *	7246119
$3p^1_{3/2}3d^1_{5/2}$	7/2(10)	6770538	$3d^2_{3/2}$	3/2(32) *	7253388
$3p^1_{1/2}3d^1_{5/2}$	3/2(20)	6771678	$3d^1_{3/2}3d^1_{5/2}$	3/2(33) *	7263947
$3p^1_{3/2}3d^1_{5/2}$	9/2(4)	6772828	$3d^2_{3/2}$	1/2(24) *	7303627
$3p^1_{1/2}3d^1_{3/2}$	3/2(21)	6780566			

Notes. The energy-ordered level index for a given level with total angular momentum J and parity is given in parentheses. An asterisk (*) denotes odd parity configurations; the lack thereof denotes an even parity configuration. The full set of energy levels is available in the online version of Table 1.

Among the total of 1784 CSFs of $\mathcal{J} = 1/2 - 11/2$, there were 909 even-parity and 875 odd-parity CSFs, which were included in the CI calculations. The MR-CI accounts for near degeneracy in energy levels, or non-dynamic correlation, inherent in multi-valence-electron systems. Frequency-independent Breit correlation corrections were included in second order, while the frequency-dependent Breit interaction ($\Delta B(\omega)$), normal mass shift, and specific mass shift are evaluated as the first order corrections using the eigenvectors $\psi_K^{\rm CI}(\gamma_K \mathcal{J}\pi)$ from the MR-CI calculation (Vilkas & Ishikawa 2005). Although it accounts well for near degeneracy in energy, the MR-CI calculation fails to accurately account for dynamic correlations. Therefore, each of the 1784 CI eigenstates was subjected to a state-specific MR-MP refinement, which accounts for the residual dynamic correlation to second order of perturbation theory (Vilkas & Ishikawa 2004, 2005)

$$E_K^{(2)} = \sum_{IJ} C_{IK} C_{JK} \left\langle \Phi_I^{(+)}(\gamma_I \mathcal{J}\pi) | V R V | \Phi_J^{(+)}(\gamma_I \mathcal{J}\pi) \right\rangle,$$
$$I, J = 1, 2, \ldots M_{\rm CI} \left(\in \mathfrak{P}^{(+)}_{C_{IK}} \right). \quad (5)$$

Here V is the MR-MP perturbation term, and R the resolvent operator acting on the subspace spanned by the residual positive-energy space $\mathfrak{Q}^{(+)} = \mathfrak{D}^{(+)} - \mathfrak{P}^{(+)}$ defined previously by Vilkas & Ishikawa (2005).

To accurately determine the effects of relativity on electron correlation, all electrons (valence and core electrons) are included in the MR-MP perturbation theory calculations. Radiative corrections were estimated for each state by evaluating the electron self-energy and vacuum polarization following an approximation scheme discussed by Indelicato et al. (1987). The code used by Indelicato et al. (1987) and Kim & Elton (1990) was modified to include our basis set expansion calculations, in order to analytically evaluate all the radial integrals. The screening of the self-energy is estimated using the ratio method by integrating the charge density of a spinor to a short distance from the origin, usually 0.3 Compton wavelengths. The ratio of the integral calculated with an MCDFB SCF spinor and the integral obtained from the analogous hydrogenic spinor is used to scale the self-energy correction for a bare nuclear charge that has been calculated by Mohr (1992).

The large and small radial components of the Dirac spinors were expanded in sets of even-tempered Gaussian-type

Table 3
Energies (in cm^{-1}) of the First 99 MR-MP Calculated Core Configurations $1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^3 3\ell^p 3\ell'^q$, ($\ell \leqslant 2$, and $p+q=2$) in Fe XVI

Configuration	J(Index)Parity	Energy	Configuration	J(Index)Parity	Energy	Configuration	J(Index)Parity	Energy
$3s^2$	3/2(4) *	5756556	$3s^1 3d^1_{5/2}$	7/2(7) *	6485011	$3p^1_{3/2}3d^1_{3/2}$	1/2(15)	6748420
$3s^1 3p^1_{1/2}$	3/2(4)	5953391	$3s^1 3d^1_{5/2}$	5/2(12) *	6501608	$3p^1_{3/2}3d^1_{5/2}$	3/2(19)	6749251
$3s^1 3p^1_{1/2}$	5/2(4)	5980479	$3p^2_{3/2}$	3/2(17) *	6531608	$3p^1_{3/2}3d^1_{3/2}$	9/2(5)	6771871
$3s^1 3p^1_{3/2}$	7/2(1)	5986775	$3p^1_{1/2}3d^1_{3/2}$	1/2(10)	6601400	$3p^1_{3/2}3d^1_{5/2}$	5/2(19)	6784892
$3s^1 3p^1_{1/2}$	3/2(5)	5987047	$3p^1_{1/2}3d^1_{3/2}$	3/2(11)	6608991	$3p^1_{3/2}3d^1_{3/2}$	7/2(11)	6794465
$3s^1 3p^1_{1/2}$	1/2(4)	5999543	$3p^1_{1/2}3d^1_{5/2}$	5/2(8)	6620899	$3p^1_{3/2}3d^1_{5/2}$	1/2(16)	6795392
$3s^1 3p^1_{3/2}$	5/2(5)	6011855	$3p^1_{1/2}3d^1_{5/2}$	7/2(2)	6634662	$3p^1_{3/2}3d^1_{5/2}$	3/2(24)	6812846
$3s^1 3p^1_{3/2}$	3/2(6)	6012375	$3p^1_{1/2}3d^1_{3/2}$	7/2(3)	6640658	$3p^1_{3/2}3d^1_{5/2}$	5/2(23)	6838045
$3s^1 3p^1_{3/2}$	1/2(5)	6027754	$3p^1_{1/2}3d^1_{5/2}$	9/2(1)	6641641	$3d^2_{3/2}$	1/2(15) *	7037203
$3s^1 3p^1_{3/2}$	5/2(6)	6096282	$3p^1_{1/2}3d^1_{3/2}$	5/2(9)	6645828	$3d^2_{3/2}$	3/2(20) *	7039419
$3s^1 3p^1_{3/2}$	3/2(9)	6113831	$3p^1_{3/2}3d^1_{5/2}$	11/2(1)	6646042	$3d^1_{3/2}3d^1_{5/2}$	5/2(15) *	7043009
$3p^2_{1/2}$	3/2(5) *	6269659	$3p^1_{1/2}3d^1_{3/2}$	3/2(12)	6650162	$3d^1_{3/2}3d^1_{5/2}$	7/2(9) *	7049523
$3p^1_{1/2}3p^1_{3/2}$	1/2(5) *	6271517	$3p^1_{3/2}3d^1_{3/2}$	5/2(10)	6659988	$3d^2_{5/2}$	11/2(1) *	7055594
$3p^1_{1/2}3p^1_{3/2}$	5/2(3) *	6278181	$3p^1_{3/2}3d^1_{5/2}$	7/2(4)	6660419	$3d^1_{3/2}3d^1_{5/2}$	9/2(2) *	7058175
$3p^1_{1/2}3p^1_{3/2}$	7/2(3) *	6287623	$3p^1_{1/2}3d^1_{3/2}$	1/2(11)	6664075	$3d^2_{3/2}$	7/2(10) *	7064132
$3p^1_{1/2}3p^1_{3/2}$	3/2(6) *	6291100	$3p^1_{1/2}3d^1_{5/2}$	7/2(5)	6673065	$3d^2_{3/2}$	5/2(16) *	7064629
$3p^2_{3/2}$	1/2(6) *	6307896	$3p^1_{1/2}3d^1_{3/2}$	1/2(12)	6673499	$3d^2_{5/2}$	9/2(3) *	7073220
$3p^1_{1/2}3p^1_{3/2}$	3/2(7) *	6308901	$3p^1_{3/2}3d^1_{3/2}$	3/2(13)	6678388	$3d^1_{3/2}3d^1_{5/2}$	5/2(17) *	7074576
$3p^1_{1/2}3p^1_{3/2}$	5/2(4) *	6308932	$3p^1_{3/2}3d^1_{5/2}$	9/2(2)	6684395	$3d^1_{3/2}3d^1_{5/2}$	7/2(11) *	7075094
$3p^2_{3/2}$	7/2(4) *	6314133	$3p^1_{1/2}3d^1_{5/2}$	3/2(14)	6686155	$3d^2_{3/2}$	3/2(22) *	7078209
$3p^2_{3/2}$	5/2(5) *	6315498	$3p^1_{3/2}3d^1_{5/2}$	5/2(11)	6686826	$3d^2_{5/2}$	5/2(18) *	7081804
$3p^2_{3/2}$	3/2(8) *	6368079	$3p^1_{3/2}3d^1_{5/2}$	7/2(6)	6688328	$3d^1_{3/2}3d^1_{5/2}$	3/2(23) *	7086971
$3s^1 3d^1_{3/2}$	1/2(8) *	6369713	$3p^1_{1/2}3d^1_{3/2}$	5/2(12)	6689006	$3d^1_{3/2}3d^1_{5/2}$	11/2(2) *	7091469
$3s^1 3d^1_{3/2}$	3/2(9) *	6377262	$3p^1_{3/2}3d^1_{3/2}$	3/2(15)	6696202	$3d^1_{3/2}3d^1_{5/2}$	1/2(17) *	7092704
$3s^1 3d^1_{5/2}$	9/2(1) *	6389221	$3p^1_{1/2}3d^1_{5/2}$	3/2(16)	6701502	$3d^2_{5/2}$	7/2(12) *	7099854
$3s^1 3d^1_{5/2}$	5/2(6) *	6390567	$3p^1_{3/2}3d^1_{5/2}$	9/2(3)	6701731	$3d^1_{3/2}3d^1_{5/2}$	5/2(20) *	7101485
$3s^1 3d^1_{3/2}$	7/2(5) *	6396084	$3p^1_{1/2}3d^1_{5/2}$	5/2(13)	6708959	$3d^1_{3/2}3d^1_{5/2}$	3/2(24) *	7103859
$3s^1 3d^1_{3/2}$	5/2(8) *	6404701	$3p^1_{3/2}3d^1_{5/2}$	7/2(7)	6710310	$3d^1_{3/2}3d^1_{5/2}$	7/2(13) *	7104169
$3p^2_{3/2}$	3/2(11) *	6406003	$3p^1_{3/2}3d^1_{3/2}$	5/2(14)	6712468	$3d^2_{5/2}$	1/2(18) *	7104271
$3s^1 3d^1_{3/2}$	3/2(12) *	6415660	$3p^1_{3/2}3d^1_{5/2}$	7/2(8)	6716199			
$3s^1 3d^1_{5/2}$	7/2(6) *	6421329	$3p^1_{3/2}3d^1_{3/2}$	1/2(13)	6716454			
$3s^1 3d^1_{3/2}$	1/2(10) *	6423578	$3p^1_{3/2}3d^1_{3/2}$	3/2(17)	6725873			
$3s^1 3d^1_{5/2}$	5/2(10) *	6425339	$3p^1_{3/2}3d^1_{5/2}$	5/2(15)	6727671			
$3s^1 3d^1_{5/2}$	3/2(14) *	6443091	$3p^1_{3/2}3d^1_{5/2}$	3/2(18)	6729273			
$3s^1 3d^1_{5/2}$	1/2(11) *	6455202	$3p^1_{1/2}3d^1_{5/2}$	1/2(14)	6741753			

Notes. The energy-ordered level index for a given level with total angular momentum J and parity is given in parentheses. An asterisk (*) denotes odd parity configurations; the lack thereof denotes an even parity configuration. The full set of energy levels is available in the online version of Table 1.

functions (Malli et al. 1993) that satisfy the boundary conditions associated with the finite nucleus, and are kinetically balanced (Ishikawa et al. 1991). The speed of light is taken to be 137.0359895 AU throughout this study. Even-tempered basis sets of $30s28p26d24f22g22h$ Gaussian (G) spinors for up to angular momentum $L = 5$, and $15G$ spinors for $L = 6$–10 are employed. The order of the partial-wave expansion $L_{\max}$, the highest angular momentum of the spinors included in the virtual space, is $L_{\max} = 10$ or up to 21 κ-symmetries, throughout this study. The nuclei were simulated as spheres of uniform proton charge with the radii $R(\text{bohr}) = 2.2677 \times 10^{-5} A^{1/3}$, where A is atomic mass (amu).

2.2. Radiative Transition Rates

Many-electron multipole transition operators T^{ϑ}_{JM} for the magnetic ($\vartheta = M$) multipoles may be given in second-quantized form (Grant 1974; Vilkas & Ishikawa 2003b):

$$T^{\vartheta}_{JM} = \sum_{ij} \left\langle t^{\vartheta}_{JM} \right\rangle_{ij} a^{+}_{i} a_{j}, \tag{6}$$

where $t^{\vartheta}_{JM}(\mathbf{r}, w)$ are one-particle multipole transition operators (Vilkas & Ishikawa 2003b). The absorption probability $\langle B \rangle_{K' \to K}$, per unit time of transition between states $|\psi_K(\gamma_K \mathcal{J} \pi)\rangle$ and $|\psi_{K'}(\gamma_{K'} \mathcal{J}' \pi')\rangle$ with transition energy $\Delta E = h\omega = E_{K'} - E_K$ is equal to the spontaneous emission probability $\langle A \rangle_{K' \to K}$ that could be expressed as

$$\left\langle B^{\vartheta}_{J} \right\rangle_{K \to K'} = 2\alpha\omega \frac{(2J+1)(J+1)}{(2J+1)J} \left[\left\langle T^{\vartheta}_{J} \right\rangle_{K'K} \right]^2 = \left\langle A^{\vartheta}_{J} \right\rangle_{K' \to K}. \tag{7}$$

In the lowest order of the Rayleigh–Schrödinger perturbation theory, the multipole transition amplitude between states K and K' is

$$\begin{aligned} \left\langle T^{\vartheta}_{J} \right\rangle^{(0)}_{KK'} &= \left\langle \psi_K(\gamma_K \mathcal{J} \pi) \left| T^{\vartheta}_{JM} \right| \psi_{K'}(\gamma_{K'} \mathcal{J}' \pi') \right\rangle \\ &= \sum_{IL} C_{IK} C_{LK'} \left\langle \Phi^{(+)}_{I}(\gamma_I \mathcal{J} \pi) \left| T^{\vartheta}_{JM} \right| \Phi^{(+)}_{L}(\gamma_L \mathcal{J}' \pi') \right\rangle, \end{aligned} \tag{8}$$

and using the order-by-order expressions of the perturbation series for the state approximated by the MCDF SCF wave

Table 4
Energies (in cm^{-1}) of the First 63 MR-MP Calculated Core Configurations $1s^2 2s^1 2p^6 3\ell^p 3\ell'^q$, ($\ell \leqslant 2$, and $p+q=2$) in Fe XVI

Configuration	J(Index)Parity	Energy	Configuration	J(Index)Parity	Energy
$3s^2$	1/2(19)	686167	$3p^1_{1/2}3d^1_{3/2}$	3/2(39) *	776849
$3s^1 3p^1_{1/2}$	1/2(16) *	705890	$3p^1_{1/2}3d^1_{5/2}$	5/2(31) *	777015
$3s^1 3p^1_{1/2}$	3/2(21) *	706508	$3p^1_{3/2}3d^1_{5/2}$	7/2(19) *	777016
$3s^1 3p^1_{3/2}$	5/2(19) *	707814	$3p^1_{3/2}3d^1_{5/2}$	7/2(20) *	778082
$3s^1 3p^1_{1/2}$	1/2(19) *	711691	$3p^1_{3/2}3d^1_{3/2}$	1/2(28) *	778131
$3s^1 3p^1_{3/2}$	3/2(26) *	712894	$3p^1_{3/2}3d^1_{3/2}$	3/2(40) *	778150
$3s^1 3p^1_{3/2}$	1/2(22) *	719926	$3p^1_{3/2}3d^1_{5/2}$	5/2(32) *	778160
$3s^1 3p^1_{3/2}$	3/2(31) *	720390	$3p^1_{1/2}3d^1_{5/2}$	3/2(41) *	781009
$3p^2_{1/2}$	1/2(22)	737454	$3p^1_{3/2}3d^1_{3/2}$	1/2(30) *	781966
$3p^1_{1/2}3p^1_{3/2}$	5/2(26)	738118	$3p^1_{3/2}3d^1_{5/2}$	5/2(33) *	782294
$3p^1_{1/2}3p^1_{3/2}$	3/2(29)	738231	$3p^1_{3/2}3d^1_{3/2}$	3/2(42) *	782330
$3p^1_{1/2}3p^1_{3/2}$	3/2(30)	738656	$3p^1_{3/2}3d^1_{3/2}$	5/2(34) *	786552
$3p^2_{3/2}$	5/2(27)	740180	$3p^1_{3/2}3d^1_{3/2}$	7/2(21) *	786616
$3p^1_{1/2}3p^1_{3/2}$	1/2(23)	740804	$3p^1_{3/2}3d^1_{5/2}$	3/2(43) *	787956
$3p^2_{3/2}$	3/2(31)	742566	$3p^1_{3/2}3d^1_{5/2}$	1/2(31) *	788162
$3s^1 3d^1_{3/2}$	1/2(24)	747313	$3d^2_{3/2}$	3/2(53)	811940
$3s^1 3d^1_{3/2}$	3/2(32)	747367	$3d^1_{3/2}3d^1_{5/2}$	5/2(46)	812044
$3s^1 3d^1_{5/2}$	5/2(28)	747465	$3d^1_{3/2}3d^1_{5/2}$	7/2(24)	812189
$3s^1 3d^1_{5/2}$	7/2(14)	747620	$3d^2_{5/2}$	9/2(10)	812375
$3p^2_{3/2}$	1/2(25)	749128	$3d^2_{3/2}$	1/2(38)	815739
$3s^1 3d^1_{3/2}$	3/2(33)	753797	$3d^1_{3/2}3d^1_{5/2}$	3/2(54)	815817
$3s^1 3d^1_{5/2}$	5/2(29)	754022	$3d^1_{3/2}3d^1_{5/2}$	5/2(47)	815884
$3s^1 3d^1_{5/2}$	3/2(34)	758386	$3d^2_{3/2}$	5/2(50)	817467
$3s^1 3d^1_{3/2}$	5/2(30)	758393	$3d^2_{5/2}$	3/2(57)	817485
$3p^1_{1/2}3d^1_{3/2}$	3/2(36) *	770952	$3d^1_{3/2}3d^1_{5/2}$	9/2(11)	817775
$3p^1_{1/2}3d^1_{3/2}$	5/2(28) *	771392	$3d^1_{3/2}3d^1_{5/2}$	5/2(51)	817787
$3p^1_{1/2}3d^1_{5/2}$	7/2(18) *	772146	$3d^1_{3/2}3d^1_{5/2}$	7/2(26)	817820
$3p^1_{3/2}3d^1_{5/2}$	9/2(7) *	773166	$3d^2_{5/2}$	7/2(27)	818014
$3p^1_{1/2}3d^1_{5/2}$	5/2(29) *	774048	$3d^1_{3/2}3d^1_{5/2}$	1/2(44)	821528
$3p^1_{3/2}3d^1_{3/2}$	3/2(37) *	774395	$3d^1_{3/2}3d^1_{5/2}$	3/2(62)	821860
$3p^1_{1/2}3d^1_{5/2}$	5/2(30) *	775849	$3d^2_{5/2}$	1/2(48)	826485
$3p^1_{1/2}3d^1_{3/2}$	1/2(27) *	776843			

Notes. The energy-ordered level index for a given level with total angular momentum J and parity is given in parentheses. An asterisk (∗) denotes odd parity configurations; the lack thereof denotes an even parity configuration. The full set of energy levels is available in the online version of Table 1.

function $\psi_K(\gamma_K \mathcal{J}\pi)$ of Equation (2), the next-order transition amplitude is

$$\left\langle T^{\vartheta}_J \right\rangle^{(1)}_{KK'} = \left\langle \psi^{(1)}_K(\gamma_K \mathcal{J}\pi) \left| T^{\vartheta}_{JM} \right| \psi_{K'}(\gamma_{K'} \mathcal{J}'\pi') \right\rangle + \left\langle \psi_K(\gamma_K \mathcal{J}\pi) \left| T^{\vartheta}_{JM} \right| \psi^{(1)}_{K'}(\gamma_{K'} \mathcal{J}'\pi') \right\rangle, \quad (9)$$

where the first-order wave function is defined as

$$\left| \psi^{(1)}_K(\gamma_K \mathcal{J}\pi) \right\rangle = RV \left| \psi_K(\gamma_K \mathcal{J}\pi) \right\rangle . \quad (10)$$

The first-order transition amplitude can be expressed in terms of CSFs in the following way:

$$\left\langle T^{\vartheta}_J \right\rangle^{(1)}_{KK'} = \sum_{L=M+1}^{\mathfrak{Q}(\pm)} \sum_{I,I'=1}^{\mathfrak{P}(+)} C_{IK} C_{I'K'} \times \left[\frac{VT_{JM}}{E^{\rm CSF}_I - E^{\rm CSF}_L} + \frac{T_{JM}V'}{E^{\rm CSF}_{I'} - E^{\rm CSF}_L} \right] \quad (11)$$

where $VT_{JM} = \langle \Phi^{(+)}_I | T^{\vartheta}_{JM} | \Phi'^{(\pm)}_{I'} \rangle \langle \Phi^{(\pm)}_I | T^{\vartheta}_{JM} | \Phi'^{(+)}_{I'} \rangle$ and $T_{JM}V' = \langle \Phi^{(+)}_I | T^{\vartheta}_{JM} | \Phi'^{(\pm)}_L \rangle \langle \Phi'^{(\pm)}_L | V | \Phi'^{(+)}_{I'} \rangle$. Summation L over intermediate states $\Phi^{(\pm)}_L$ includes both the positive $\mathfrak{Q}^{(+)}$ and negative $\mathfrak{Q}^{(-)}$ energy subspaces (Johnson et al. 1995). With the summation extended to negative-energy sub-space, the $E1$ transition probability is computed in the length gauge. One-electron reduced matrix elements are frequency dependent through the spherical Bessel functions $j_J(kr)$. The corrections arising from approximate photon frequencies may be eliminated semiempirically using experimental transition energies. The radiative E1 transition probabilities were calculated using both the CI method and the MR-MP perturbation theory approach.

3. RESULTS AND DISCUSSION

We have calculated the energies of the ground and a number of even- and odd-parity excited states of sodium-like iron by state-averaged MCDF followed by relativistic multireference many-body perturbation theory. The numbers of CSFs generated were, respectively, 154, 236, 232, 163, 89 and 35 for the $J = \{1/2,\ 3/2,\ 5/2,\ 7/2,\ 9/2,\ 11/2\}$ even-parity states, while for the odd-parity is $J = \{1/2,\ 3/2,\ 5/2,\ 7/2,\ 9/2,\ 11/2\}$ states they were, respectively, 150, 232, 223, 159, 81 and 30 CSFs. All these CSFs were included in the state-averaged energy Equation (1).

The large amount of levels (1784) precludes us from including all in this paper. However, the full set of energy levels calculated by our methods is given in the online material. In the following, we discuss a representative subset of our calculations, which includes most of the lines that might be of importance to the modeling of astrophysical plasmas.

In Table 1 we list the energies of the first 18 singly excited levels up to $5f^1_{7/2}$. Our calculations can be compared to the energy level data compiled by NIST (Kramida et al. 2012). The differences are small for the low-lying levels, but for levels with electrons in the $n = 5$ shell the difference increase to 1300 cm^{-1}. Such discrepancies indicate that some levels might be not well allocated or identified. The first four entries can also be compared to the previous MR-MP calculations (Beiersdorfer et al. 2011). The difference between these two calculations is less than 20 cm^{-1}. Doschek & Feldman (2010) list four Fe XVI lines that have been observed in the Sun. These are located at 360.8 Å, 335.41 Å, 251.06 Å, and 262.97 Å. The first two connect the upper $1s^2 2s^2 2p^6 3p^o_{1/2}$ and $1s^2 2s^2 2p^6 3p^o_{3/2}$ levels directly to the $1s^2 2s^2 2p^6 3s$ ground state. Our calculations predict 360.72 Å and 335.38 Å, respectively, for these lines. The other two lines correspond to the $3d_{3/2} \rightarrow 3p^o_{1/2}$ and $3d_{5/2} \rightarrow 3p^o_{3/2}$ transitions, for which we obtain 251.10 Å and 263.02 Å, respectively. Our predictions thus agree to within 0.08 Å with the solar data.

In Tables 2, 3, and 4 we present energy levels for the core-excited configurations $2s^2 2p^1_{1/2} 2p^4_{1/2}$, $2s^2 2p^2_{1/2} 2p^3_{3/2}$, and $2s^1 2p^2_{1/2} 2p^4_{3/2}$, respectively, and two valence electrons in the $n = 3$ shell up to $3d^2_{5/2}$. Tables 2 and 3 list 67 and 99 levels, respectively, while Table 4 list the first 63 levels that contain up to $3d^2_{5/2}$ excitations.

In Table 5 comparisons are made with RMBPT results calculated by Safronova et al. (2002a) for Na-like iron core-excited states as a theoretical benchmark. The comparison reveals differences as large as 3000 cm^{-1}. We point out that the two methods do not always agree on the dominant CSF for describing a given level.

At present, the NIST Atomic Database lists 34 Fe XVI core-excited states. They have identified a total of six levels as a blend of several decays. The first four blend levels are $(2p^5 3s 3p)_{J=3/2}$,

Table 5
Comparison of Core-excited States Calculated with RMBPT and MR-MP

RMBPT Configuration	J(Index)	$E_{\text{MR-MP}}$[a]	E_{RMBPT}[b]	ΔE	MR-MP Configuration
Core $1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^3 3s$					
$3p_{1/2}$	3/2(4)	5953391	5955393	−2002	
$3p_{1/2}$	5/2(4)	5980479	5979729	750	
$3p_{3/2}$	7/2(1)	5986775	5986121	654	
$3p_{1/2}$	3/2(5)	5987047	5986183	864	
$3p_{1/2}$	1/2(4)	5999543	5996901	2642	
$3p_{3/2}$	3/2(6)	6012375	6010900	1475	
$3p_{3/2}$	5/2(5)	6011855	6011138	717	
$3p_{3/2}$	1/2(5)	6027754	6027666	88	
$3p_{3/2}$	1/2(6)	6077192	6076276	916	$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s 3p_{1/2}$
$3p_{3/2}$	3/2(7)	6087509	6086743	766	$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s 3p_{1/2}$
$3p_{3/2}$	5/2(6)	6096282	6095011	1271	
Core $1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s$					
$3p_{1/2}$	1/2(7)	6082835	6082503	332	
$3p_{1/2}$	3/2(8)	6100268	6098145	2123	$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s 3p_{3/2}$
$3p_{3/2}$	5/2(7)	6108077	6107484	593	
$3p_{3/2}$	3/2(9)	6113831	6112414	1417	$1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^3 3s 3p_{3/2}$
$3p_{1/2}$	1/2(8)	6182346	6180904	1442	$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s 3p_{3/2}$
$3p_{3/2}$	3/2(10)	6201702	6200281	1421	
$3p_{3/2}$	1/2(9)	6245187	6246108	−921	$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s 3p_{1/2}$

Notes. All excited states decay to the $1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^4 3s\ J = 1/2$ ground level. All energies are given in (cm^{-1}). The energy-ordered level index for a given level with total angular momentum J is given in parentheses.
[a] Present calculation.
[b] Safronova et al. (2002a).

$(2p^5 3s 3p)_{J=5/2}$, $(2p^5 3s 3p)_{J=1/2}$ and $(2p^5 3s 3p)_{J=3/2}$. They reported the same energy value for the following configurations $2p^5 3s 3p$ with $J = \{3/2, 5/2\}$ as 6,013,000 cm^{-1} and for $2p^5 3s 3p$ with $J = \{1/2, 3/2\}$ as 6,089,000 cm^{-1}. When compared to our theoretical calculation with the blended levels $(2p^5 3s 3p)_{J=3/2,5/2}$ given by NIST each level differs by 520 cm^{-1} and 4674 cm^{-1}, respectively. The next two blended levels $(2p^5 3s 3d)_{J=3/2,5/2}$ have as much as 2000 cm^{-1} of difference between each level. Our MR-MP calculations show a significant energy separation between these blended levels that is not reflected in data compiled by NIST, suggesting the need for a precise method to correctly assign each of these energy levels. We know due to the large amount of possible transitions is very difficult to make correct identifications. Our data should allow an update of these assignments.

In Table 6 we list the energies and line identifications for Fe XVI transitions provided by two recent laboratory measurements (Brown et al. 2001; Graf et al. 2009). A comparison of the laboratory measurements with our calculations shows excellent agreement. In some cases, where a measured feature is a blend of multiple lines, the calculated wavelength of the strongest contribution is in agreement with the measured wavelength. The table also compares the values for the upper and lower level energies and the transition wavelengths obtained with our earlier, smaller MR-MP calculation involving core excitation only up to $n = 3$ (Beiersdorfer et al. 2012) with our present calculation involving core excitation up to $n = 5$. When including the 4ℓ and 5ℓ ($\ell = s, p, d, f$) configurations to get a better description of the system, additional 1542 levels are generated. The larger calculation produces wavelengths that differ from the ones calculated with the smaller set of levels by about 0.002 Å. This difference cannot be resolved within the measurement error.

In Table 7 we compare our values for four Fe XVI lines with those obtained from various solar observations and laboratory measurements. The line at 17.598 Å was measured by Burkhalter et al. (1979) using a laser source (ls) and a vacuum spark (vs) getting very close values with a difference of 3 mÅ. Then, Acton et al. (1985) used solar flare (sf) observations to determine the same line, obtaining a deviation of 4 mÅ compared with Burkhalter's laboratory value. The Fe XVI line at 17.500 Å was studied several times employing different methods. First, by Burkhalter et al. using vs and ls, who achieved very good agreement, within 1 mÅ, with his calculated theoretical value of 17.500 Å. This was followed by Phillips et al. (1982) and Acton et al. (1985). They obtained 17.496 Å and 17.494 Å, respectively. The theoretical calculation for the line at 17.212 Å made by Burkhalter et al. (1979) overestimated the values determined experimentally by 170–190 mÅ. Subsequently Phillips et al. (1982) obtained a lower value (17.203 Å); some years later they repeated the measurement and obtained a result that agreed with Burkhalter's experimental value within 4 mÅ. Although Burkhalter et al. (1979) could establish from their theoretical calculation that satellite lines occur mainly in the 15.1–15.6 Å region, the agreement with the observation was not sufficient to identify the line at 15.212 Å. This line was observed by Phillips et al. (1982) in solar flare observations, allowing them to resolve many line blends for the first time. Three years later, Acton et al. (1985) observed the same line (15.21 Å) using a high resolution (0.02 Å) rocket-borne spectrograph obtaining a slight improvement in the measurements. When comparing our calculated values to each of the four lines in Table 7 with the values measured in solar flare observation, we find that they are very similar, with a difference of $\leqslant$0.006 Å.

In Table 8 we list the results from May et al. (2005) who used the Hebrew University Lawrence Livermore Atomic Code (HULLAC) and FAC codes to calculate the Fe XVI atomic structure and wavelengths. The table also lists the Fe XVI experimental wavelengths they obtained from a laser-produced

Table 6
Comparison of Calculated and Measured Wavelengths of Innershell Excited Fe XVI Transitions

Label	λ_{exp}[a] (Å)	Upper Level	Lower Level	λ[b] (Å)	$\|\lambda^b - \lambda_{exp}\|$	Upper Level	Lower Level	λ[c] (Å)	$\|\lambda^c - \lambda_{exp}\|$	Identification[c]
1	15.11	6618026	0	15.110	0.000	6616740	0	15.113	0.003	$(2p^6 3s)_{J=1/2} - (2p_{1/2}2p^4_{3/2}3s3d_{5/2})_{J=3/2}$
2a	15.19	6879647	298162	15.194	0.004	6878831	298167	15.196	0.002	$(2p^6 3p_{3/2})_{J=3/2} - (2s_{1/2}2p^6 3s^2)_{J=1/2}$
2b	15.21	6574091	0	15.211	0.001	6573657	0	15.212	0.001	$(2p^6 3s)_{J=1/2} - (2p_{1/2}2p^4_{3/2}3s3d_{3/2})_{J=1/2}$
3	15.261	6550663	0	15.266	0.005	6550184	0	15.267	0.001	$(2p^6 3s)_{J=1/2} - (2p_{1/2}2p^4_{3/2}3s3d_{5/2})_{J=3/2}$
4	15.516	6444071	0	15.518	0.002	6443091	0	15.521	0.003	$(2p^6 3s)_{J=1/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{5/2})_{J=3/2}$
5	15.679	6378202	0	15.678	0.001	6377262	0	15.681	0.003	$(2p^6 3s)_{J=1/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{3/2})_{J=3/2}$
6a	17.371	5756768	0	17.371	0.000	5756556	0	17.371	0.000	$(2p^6 3s)_{J=1/2} - (2p^2_{1/2}2p^3_{3/2}3s^2)_{J=3/2}$
6b	17.395	6426192	678378	17.398	0.003	6425339	678372	17.400	0.002	$(2p^6 3d_{5/2})_{J=5/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{5/2})_{J=5/2}$
		6422857	675468	17.399		6422064	675463	17.402	0.003	$(2p^6 3d_{3/2})_{J=3/2} - (2p_{1/2}2p^4_{3/2}3p^2_{3/2})_{J=3/2}$
6c	17.417	6422017	678378	17.411	0.006	6421329	678372	17.413	0.002	$(2p^6 3d_{5/2})_{J=5/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{5/2})_{J=7/2}$
		6416429	675468	17.419		6415660	675463	17.421	0.002	$(2p^6 3d_{3/2})_{J=3/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{3/2})_{J=3/2}$
7	17.447	6012856	277210	17.435	0.012	6012375	277222	17.436	0.001	$(2p^6 3p_{1/2})_{J=1/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{3/2})_{J=3/2}$
		6405477	675468	17.452		6404701	675463	17.454	0.002	$(2p^6 3d_{3/2})_{J=3/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{3/2})_{J=5/2}$
		6028419	298162	17.451		6027754	298167	17.453	0.002	$(2p^6 3p_{3/2})_{J=3/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{3/2})_{J=1/2}$
8a	17.494	6000073	277210	17.474	0.020	5999543	277222	17.475	0.001	$(2p^6 3p_{1/2})_{J=1/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{1/2})_{J=1/2}$
		6396885	678378	17.487		6396084	678372	17.490	0.003	$(2p^6 3d_{5/2})_{J=5/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{3/2})_{J=7/2}$
		6394828	678378	17.493		6394058	678372	17.496	0.003	$(2p^6 3d_{5/2})_{J=5/2} - (2p^2_{1/2}2p^3_{3/2}3s3d_{5/2})_{J=5/2}$
		6012856	298162	17.499		6012375	298167	17.500	0.001	$(2p^6 3p_{3/2})_{J=3/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{3/2})_{J=3/2}$
		6012318	298162	17.500		6011855	298167	17.502	0.002	$(2p^6 3p_{3/2})_{J=3/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{3/2})_{J=5/2}$
8b	17.51	5987547	277210	17.512	0.002	5987047	277222	17.514	0.002	$(2p^6 3p_{1/2})_{J=1/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{1/2})_{J=3/2}$
9a	17.592	5980999	298162	17.597	0.005	5980479	298167	17.598	0.001	$(2p^6 3p_{3/2})_{J=3/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{1/2})_{J=5/2}$
9b	17.612	5954207	277210	17.615	0.003	5953391	277222	17.618	0.003	$(2p^6 3p_{1/2})_{J=1/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{1/2})_{J=3/2}$
10	17.678	5954207	298162	17.680	0.002	5953391	298167	17.683	0.003	$(2p^6 3p_{3/2})_{J=3/2} - (2p^2_{1/2}2p^3_{3/2}3s3p_{1/2})_{J=3/2}$

Notes.
[a] From Graf et al. (2009).
[b] From previous work (Beiersdorfer et al. 2011).
[c] This work.

Table 7
Comparison of MR-MP Calculated Fe XVI Wavelengths with Solar Flare (sf), Vacuum Spark (vs), and Laser-source (ls) Measurements

Transition	λ_{exp}[a] (sf)	λ_{exp}[b] (sf)	λ_{exp}[c] (sf)	λ_{exp}[d] (vs)	λ_{exp}[d] (ls)	λ_{theory}[d]	λ_{MRMP}
$(2p^6 3p_{3/2})_{J=3/2} \rightarrow (2p^2_{1/2}2p^3_{3/2}3s_{1/2}3p_{1/2})_{J=5/2}$			17.592	17.593	17.596	17.604	17.598
$(2p^6 3p_{3/2})_{J=3/2} \rightarrow (2p^2_{1/2}2p^3_{3/2}3s_{1/2}3p_{3/2})_{J=3/2}$	17.496	17.500	17.494	17.498	17.499	17.500	17.500
$(2p^6 3p_{3/2})_{J=3/2} \rightarrow (2p_{1/2}2p^4_{3/2}3s_{1/2}3p_{3/2})_{J=5/2}$	17.203	17.210		17.206	17.208	17.225	17.212
$(2p^6 3s)_{J=1/2} \rightarrow (2p_{1/2}2p^4_{3/2}3s_{1/2}3d_{3/2})_{J=1/2}$	15.205		15.21				15.212

Notes. Also listed are theoretical wavelengths from Burkhalter et al. (1979). All values are in Å.
[a] Phillips et al. (1982).
[b] Phillips et al. (1999).
[c] Acton et al. (1985).
[d] Burkhalter et al. (1979).

plasma source. In general, our theoretical results are in better agreement with their experimental values than the values they obtained from HULLAC calculations. In addition, we found three lines identified by May et al. (2005), 15.500 Å, 15.360 Å, and 15.087 Å, in which the configuration for the upper level determined by HULLAC differs from our MR-MP calculations.

From Table 8 we can see there are many discrepancies between our calculated and the experimental values. Based on the accuracy of our method ascertained in comparisons with experimental and solar observations in Tables 6 and 7, where we find differences equal to or less than 0.006 Å, we believe that the lines for which the difference are larger than 0.010 mÅ are not correctly identified or that the experimental errors are much larger than assumed. This illustrates the need to employ more accurate theoretical wavelengths than those produced by the HULLAC code to help with line identification.

In Table 9 we list the radiative rates (A_r in s^{-1}) we calculated for electric dipole (E1) transitions in the 15.02–15.27 Å range. This is the region containing the strongest Fe XVI lines. Also radiative branching ratio defined by ($\beta = \tau A_r$) are included, where the lifetime τ is defined as $\tau = 1/\sum A_r$. These calculations were made using both the CI and the MR-MP approach. The comparison shows that the two methods produce results that agree within 8%. This suggest, that it is sufficient to employ the CI method for calculating radiative rates, as such rates typically are not needed with a high accuracy. This is especially important to note because a lot fewer computer resources and time are needed for the CI method than for the MR-MP method.

Table 8
Comparison of Our Theoretical Method (MR-MP) with Other Experimental and Theoretical Calculation in the Range of 13.938–15.500 Å

	λ_{exp}	λ_{HUL}	$\lambda_{MR\text{-}MP}$	$\Delta\lambda_{HUL}$	$\Delta\lambda_{MR\text{-}MP}$	Transition	Suggest Upper Level
Na1b	15.500	15.4562	15.5013	−0.0438	0.0013	$2s^22p_{1/2}2p^4_{3/2}3p_{1/2}3d_{5/2} \rightarrow 2s^22p^63p_{3/2}$	$2s^22p^2_{1/2}2p^3_{3/2}3p_{3/2}3d_{5/2}$
Na2b	15.360	15.3534	15.3595	−0.0066	−0.0005	$2s^22p_{1/2}2p^4_{3/2}3d^2_{3/2} \rightarrow 2s^22p^63d_{3/2}$	$2s^22p_{1/2}2p^4_{3/2}3d_{3/2}3d_{5/2}$
Na3	15.304	15.2899	15.2908	−0.0141	−0.0132	$2s^22p^2_{1/2}2p^3_{3/2}3p_{3/2}3d_{5/2} \rightarrow 2s^22p^63p_{3/2}$	
Na4	15.290	15.2687	15.2667	−0.0213	−0.0233	$2s^22p_{1/2}2p^4_{3/2}3s3d_{5/2} \rightarrow 2s^22p^63s$	
Na5	15.276	15.2552	15.2577	−0.0208	−0.0183	$2s^22p_{1/2}2p^4_{3/2}3p_{1/2}3d_{3/2} \rightarrow 2s^22p^63p_{1/2}$	
		15.2427	15.2411			$2s^22p_{1/2}2p^4_{3/2}3p_{3/2}3d_{3/2} \rightarrow 2s^22p^63p_{3/2}$	
Na6	15.237	15.2247	15.2259	−0.0123	−0.0111	$2s^22p_{1/2}2p^4_{3/2}3d_{3/2}3d_{5/2} \rightarrow 2s^22p^63d_{5/2}$	
Na7	15.213	15.2364	15.2336	0.0234	0.0206	$2s^22p_{1/2}2p^4_{3/2}3d_{3/2}3d_{5/2} \rightarrow 2s^22p^63d_{5/2}$	
Na8	15.174	15.2081	15.2122	0.0341	0.0382	$2s^22p_{1/2}2p^4_{3/2}3s3d_{3/2} \rightarrow 2s^22p^63s$	
		15.200	15.2024			$2s^22p_{1/2}2p^4_{3/2}3d^2_{3/2} \rightarrow 2s^22p^63d_{3/2}$	
Na9	15.159	15.1601	15.1729	0.0011	0.0139	$2s^22p_{1/2}2p^4_{3/2}3p_{3/2}3d_{3/2} \rightarrow 2s^22p^63p_{3/2}$	
Na10	15.087	15.0996	15.1132	0.0126	0.0262	$2s^22p_{1/2}2p^4_{3/2}3p_{1/2}3p_{3/2} \rightarrow 2s^22p^63s$	$2s^22p_{1/2}2p^4_{3/2}3s3d_{3/2}$
Na11	15.064	15.0768	15.0718	0.0128	0.0078	$2s^22p_{1/2}2p^4_{3/2}3d_{3/2}4d_{5/2} \rightarrow 2s^22p^64d_{5/2}$	
Na12	15.031	15.0743	15.0734	0.0433	0.0424	$2s^22p_{1/2}2p^4_{3/2}3d_{3/2}4f_{5/2} \rightarrow 2s^22p^64f_{5/2}$	
		15.0081	15.0244			$2s^22p_{1/2}2p^4_{3/2}3d_{3/2}4f_{7/2} \rightarrow 2s^22p^64f_{7/2}$	
Na13b	14.097	14.0893	14.1183	−0.0077	0.0213	$2s2p^63p_{1/2}3p_{3/2} \rightarrow 2s^22p^63p_{3/2}$	
Na14b	14.093	14.0866	14.0951	−0.0064	0.0021	$2s2p^63p_{1/2}3d_{5/2} \rightarrow 2s^22p^63d_{3/2}$	
Na15	14.060	14.0688	14.0796	0.0088	0.0196	$2s2p^63p_{3/2}3d_{5/2} \rightarrow 2s^22p^63d_{5/2}$	
Na16	14.018	14.0161	14.0510	−0.0019	0.0330	$2s2p^63s3p_{1/2} \rightarrow 2s^22p^63s$	
Na17	13.938	13.9979	14.0302	0.0599	0.0922	$2s2p^63p^2_{3/2} \rightarrow 2s^22p^63p_{3/2}$	

Note. A "b" after the label indicates a blend.

Table 9
Theoretical Radiative Transition Rates (A_r in $\times 10^{12}$ s^{-1}) and Radiative Branching Ratios ($\beta = \tau A_r$) of E1 Transitions Situated between 15.016 Å and 15.267 Å

λ	Upper	Lower	$A_r^{MR\text{-}MP}$	A_r^{CI}	β^{CI}	λ	Upper	Lower	$A_r^{MR\text{-}MP}$	A_r^{CI}	β^{CI}
15.01589	3/2(127)	5/2(1)*	17.4735	18.555	17.486	15.04945	5/2(181)*	5/2(3)	11.8143	12.180	6.330
15.02439	9/2(44)	7/2(1)*	14.5907	14.431	12.902	15.04994	5/2(180)*	3/2(3)	11.7651	12.118	6.330
15.02456	5/2(122)	7/2(1)*	16.5394	17.611	13.329	15.05153	5/2(180)*	5/2(3)	9.8140	10.179	4.466
15.02495	3/2(202)	5/2(2)*	21.1736	22.163	21.582	15.05169	3/2(118)*	5/2(2)	11.3624	11.826	6.917
15.01589	3/2(127)	5/2(1)*	17.4735	18.555	17.486	15.06017	1/2(66)	3/2(2)*	16.7163	17.439	14.110
15.02439	9/2(44)	7/2(1)*	14.5907	14.431	12.902	15.06410	3/2(117)*	3/2(2)	11.4402	11.715	6.489
15.02456	5/2(122)	7/2(1)*	16.5394	17.611	13.329	15.06659	3/2(88)*	1/2(2)	20.6732	21.428	20.977
15.02495	3/2(202)	5/2(2)*	21.1736	22.163	21.582	15.06901	3/2(95)	1/2(2)*	10.9642	11.389	6.148
15.02664	5/2(199)	7/2(2)*	18.7308	19.626	16.511	15.06911	1/2(58)*	1/2(2)	20.8456	21.644	21.140
15.03163	9/2(77)	7/2(2)*	20.2544	20.394	19.706	15.07033	5/2(89)	3/2(2)*	19.9536	20.697	20.356
15.03385	5/2(198)	5/2(2)*	18.4600	19.064	15.870	15.07184	7/2(75)*	5/2(2)	17.8116	17.817	17.310
15.03702	7/2(139)	7/2(2)*	21.5995	22.286	21.589	15.07336	7/2(81)	5/2(1)*	21.9747	21.962	21.065
15.03915	1/2(78)*	3/2(2)	10.0347	10.403	9.841	15.07357	1/2(65)	1/2(2)*	14.3686	14.868	11.181
15.04078	3/2(190)*	5/2(3)	16.0079	16.544	12.029	15.07652	5/2(109)*	5/2(2)	18.6489	19.209	17.935
15.04079	1/2(125)	3/2(3)*	17.7654	18.351	14.821	15.07935	3/2(96)	3/2(2)*	11.5953	12.036	6.763
15.04109	5/2(121)	5/2(1)*	15.4934	16.057	11.544	15.09053	5/2(108)*	3/2(2)	21.6734	22.480	20.002
15.04273	1/2(124)*	3/2(3)	20.8246	21.375	21.079	15.18470	3/2(33)*	5/2(1)	12.5156	13.359	8.179
15.04296	1/2(114)*	1/2(3)	21.3543	22.017	21.732	15.19603	1/2(20)	3/2(1)*	15.1096	16.129	15.858
15.04391	3/2(186)	1/2(3)*	14.7197	15.201	10.474	15.20236	3/2(32)*	3/2(1)	15.8994	16.924	11.567
15.04406	3/2(176)*	1/2(3)	21.0601	21.690	21.416	15.21223	1/2(14)*	1/2(1)	22.5016	23.696	23.190
15.04445	7/2(138)	5/2(2)*	22.2837	22.479	21.960	15.22592	5/2(26)*	5/2(1)	22.4512	23.844	23.496
15.04578	3/2(189)*	3/2(3)	15.5917	16.119	11.358	15.23358	7/2(17)*	5/2(1)	12.3671	12.251	12.219
15.04583	7/2(128)*	5/2(3)	21.4781	21.824	21.378	15.23373	1/2(18)	1/2(1)*	14.0857	14.967	14.775
15.04629	5/2(182)	3/2(3)*	21.2787	22.045	21.816	15.24108	3/2(26)	3/2(1)*	16.2215	17.227	16.934
15.04786	5/2(181)*	3/2(3)	10.0889	10.305	4.531	15.24287	1/2(23)*	3/2(1)	11.9933	12.803	12.719
15.04814	1/2(124)	1/2(3)*	17.3439	17.886	14.335	15.25772	3/2(25)	1/2(1)*	17.7356	18.784	18.437
15.04898	7/2(82)	7/2(1)*	20.0305	20.775	19.500	15.26675	3/2(18)*	1/2(1)	13.1244	14.296	13.777

Notes. The energy-ordered level index for a given upper or lower level with total angular momentum J and parity is given in parentheses. An asterisk (∗) denotes odd parity configurations; the lack thereof denotes an even parity configuration. Only transition with $A_r \geqslant 10^{12}$ s^{-1} are listed. $A_r^{MR\text{-}MP}$ denotes rates calculated with the MR-MP method; A_r^{CI} and β^{CI} were calculated with the CI method. The full set of radiative rates for transitions between 10.374 and 15.469 Å is available in the online version of Table 9.

(This table is available in its entirety in a machine-readable form in the online journal. A portion is shown here for guidance regarding its form and content.)

Table 10
Comparison of Energy Levels (cm^{-1}), Wavelengths (Å), and E1 Transition Rates (A_r in $\times 10^{10}$ s^{-1}) of Core-excited States between RMBPT and MR-MP Calculations

Configuration	J	$E_{\text{MR-MP}}$	$\lambda_{\text{MR-MP}}$	λ_{RMBPT}	$\Delta\lambda$	A_r^{RMBPT}	$A_r^{\text{MR-MP}}$
$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s^2$	1/2(4)*	5857665	17.0716	17.0747	0.0031	80.96	75.310
$1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^3 3s 3d_{3/2}$	1/2(5)*	6271517	15.9451	15.9418	−0.0033	9.449	7.008
$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3p_{1/2}^2$	1/2(9)*	6398771	15.6280	15.6327	0.0047	0.253	0.10877
$1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^3 3s 3d_{3/2}$	1/2(10)*	6423578	15.5676	15.5711	0.0035	46.00	49.875
$1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^3 3s 3d_{5/2}$	1/2(11)*	6455202	15.4914	15.5029	0.0115	377.600	323.091
$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3p_{1/2} 3p_{3/2}$	1/2(13)*	6514341	15.3507	15.3681	0.0174	14.650	13.1757
$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3p_{3/2}^2$	1/2(12)*	6508883	15.3636	15.3672	0.0036	0.094	16.853
$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3s 3d_{3/2}$	1/2(14)*	6573657	15.2122	15.2148	0.0026	2240.000	2250.16
$1s^2 2s 2p_{1/2}^2 2p_{3/2}^4 3s 3p_{1/2}$	1/2(19)*	7116914	14.0510	14.0969	0.0459	2.826	255.782
$1s^2 2s^2 2p_{1/2} 2p_{3/2}^4 3d_{5/2}^2$	1/2(24)*	7303627	13.6918	13.6959	0.0041	0.009	0.02368

Notes. All excited states decay to the $1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^4 3s$ $J = 1/2$ ground level. The energy-ordered level index for a given level with total angular momentum J and parity is given in parentheses. An asterisk (∗) denotes odd parity configurations; the lack thereof denotes an even parity configuration.

We compare selected RMBPT (Safronova et al. 2002b) and MR-MP calculated energy levels and transition rates for odd-parity states decaying to the $(1s^2 2s^2 2p_{1/2}^2 2p_{3/2}^4 3s)_{J=1/2}$ ground level in Table 10. Three transitions have rates for which the results deviate by up to two orders of magnitude, i.e., those from upper levels 1/2(12)*, 1/2(19)* and 1/2(24)*. Two allowed E1 transition occupation configurations 1/2(5)* and 1/2(24)* described in Tables 3 and 2, differ from the obtained by RMBPT method. We note the wavelengths calculated by the RMPBT and MR-MP methods differ by up to 46 mÅ for the transitions shown.

4. CONCLUSION

Multiple open-shell systems with two valence electrons give rise to complex spectra because of a large number of nearly degenerate multiplet states. In an earlier study, the relativistic MR-MP perturbation theory based on the state-averaged MCDF SCF was implemented and successfully applied to silicon-like argon and for the ions of the silicon isoelectronic sequence (Vilkas & Ishikawa 2003a, 2003b). In the present study, relativistic multireference perturbation calculations have been carried out for a large number of odd- and even-parity excited levels with $n \leqslant 5$ of sodium-like iron. These calculation show that the MR-MP method can provide accurate term energies, transition energies, and transition rates for numerous excited levels of multi-valence-electron atoms.

The continuing developments in astrophysical observations demand accurate theoretical transition data to accurately determine stellar chemical compositions. Our theoretical data obtained from the highly correlated MR-MP calculations are of spectroscopic accuracy for the highly charged Na-like ion Fe XVI. The excited Fe XVI ion has a large amount of possible transitions, which makes correct line identifications difficult as illustrated by our discussion of the laser data obtained by May et al. (2005). Transition energies produced by the MR-MP method could become a useful tool for experimentalist and modelers to make line identifications and to help them to untangled blends.

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